

Trap-Assisted Tunneling in the Schottky Barrier

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Abstract. The paper presents a new way how to calculate the currents in a Schottky barrier. The novel phenomenological model extends the Shockley-Read-Hall recombination-generation theory of trap-assisted tunneling. The proposed approach explains the occurrence of large leakage currents in Schottky structures on wide band semiconductors with a high Schottky barrier (above 1 eV) and with a high density of traps. Under certain conditions, trap-assisted tunneling (TAT) plays a more important role than direct tunneling.

Keywords

Trap-assisted tunneling, direct tunneling, Schottky barrier.

1. Introduction

The main problem hindering extensive exploitation of AlGaIn/GaN high electron mobility transistors (HEMTs) are the unacceptably large gate leakage currents [1], [2]. The mechanism of leakage currents still has not been fully understood and elucidated. One of the possible reasons might be trap-assisted tunneling [3].

Trap-assisted tunneling results in a reduction of the Shockley-Read-Hall (SRH) recombination lifetimes in the regions of strong electric fields. I - V characteristics of the Schottky junction are extremely sensitive to defect-assisted tunneling. The classical SRH model assumes that intermediate trap centers with concentration N_t lie on a discrete energy level E_t . In our model we propose that – due to electron-phonon interactions – the discrete energy level E_t broadens hereby giving rise to a band of multi-phonon excitation traps.

2. Theory

The physical model of trap-assisted tunneling is based on solving the Poisson and continuity equations. In the sequel, for the sake of simplicity we will consider a Schottky barrier created on an n -type semiconductor. This allows to neglect hole tunneling. We will also assume

that deep trapping centers are of donor type (a trap unoccupied by an electron has a positive charge).

Under these assumptions the well known Poisson equation can be written as

$$-\frac{d}{dx}\left(\kappa(x)\frac{d\psi(x)}{dx}\right) = q(p(x) - n(x) + N^{D+}(x) + N_t^+(x)) \quad (1)$$

where κ is the semiconductor permittivity, ψ is the electric potential, n and p are concentrations of free charge carriers, N^{D+} is the concentration of shallow ionized donors and N_t^+ is the concentration of deep ionized donors expressed as

$$N_t^+(x) = \int_{E_V(x)}^{E_C(x)} D_t(x, \varepsilon) (1 - f_t(x, \varepsilon)) d\varepsilon. \quad (2)$$

Here, f_t is the occupation probability of trapping centers lying at deep energy level ε . Definition of the distribution functions of traps in the forbidden band, based on the theory of multiphonon assisted tunneling, is given as [4-6]

$$D_t(\varepsilon, x) = \frac{N_t}{\sqrt{2\pi}\varepsilon_r} \frac{(\theta \mp S)^2}{(\theta^2 + z^2)^{\frac{1}{4}}} \times \exp\left(\sqrt{z^2 + \theta^2} - \theta \ln\left(\frac{\theta}{z} + \sqrt{1 + \left(\frac{\theta}{z}\right)^2}\right) - S(2f_B + 1) - \frac{|\varepsilon - E_t|}{2kT}\right) \quad (3)$$

where S is the Huang-Rhys factor representing the strength of electron-phonon coupling, $\varepsilon_r = S\hbar\omega_0$ is the lattice relaxation energy, $\hbar\omega_0$ is the effective phonon energy,

$\theta = \frac{|\varepsilon - E_t|}{\hbar\omega_0}$, $f_B = \left(\exp\left(\frac{\hbar\omega_0}{kT}\right) - 1\right)^{-1}$ is the Bose distribu-

tion function, and $z = 2S\sqrt{f_B(1 + f_B)}$. The sign inside the bracket in the nominator is negative for $\varepsilon > E_C(x) - E_t$ and positive for $\varepsilon < E_C(x) - E_t$.

The continuity equations for electrons and holes can be written as

$$\frac{dJ_D^e(x)}{q dx} = U_{TAT}^{e(THER)}(x) + U_{TAT}^{e(TUN)}(x) + U_{DT}^e(x) = U^e(x), \quad (4)$$

$$-\frac{dJ_D^h(x)}{q dx} = U_{SRH}(x) \quad (5)$$

where

$$J_D^e = -q\mu^e(x) \left(n(x) \frac{d\psi(x)}{dx} - \frac{kT}{q} \frac{dn(x)}{dx} \right), \quad (6)$$

$$J_D^h = -q\mu^h(x) \left(p(x) \frac{d\psi(x)}{dx} + \frac{kT}{q} \frac{dp(x)}{dx} \right) \quad (7)$$

are the electron and hole drift-diffusion current densities.

On the right hand side of (4) there are two dominant terms $U_{TAT}^{e(THER)}$ and $U_{TAT}^{e(TUN)}$, the electron recombination rates of trap-assisted tunneling, and U_{DT}^e is the rate of direct tunneling. The right hand side of (5) contains the Shockley-Read-Hall recombination rate U_{SRH} .

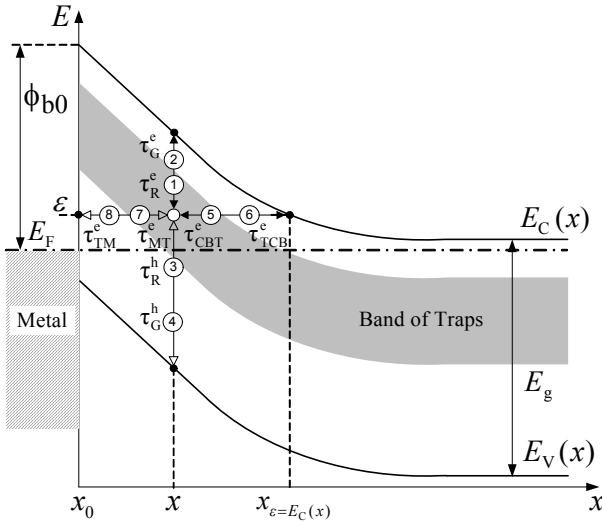


Fig. 1. Eight exchange processes involved in the new model of trap-assisted band-to-band tunneling.

The model of TAT introduces the concepts of thermal and tunneling escape times, see Fig. 1. The formulae for calculating the thermal escape times are

$$(\tau_R^e(x))^{-1} = v_{th}^e \sigma_t n(x), \quad (8)$$

$$(\tau_G^e(x))^{-1} = v_{th}^e \sigma_t N_C \exp((\varepsilon - E_C(x))/kT), \quad (9)$$

$$(\tau_R^h(x))^{-1} = v_{th}^h \sigma_t p(x), \quad (10)$$

$$U_{TAT}^{e(THER)}(x) = \int_{E_V(x_s)}^{E_C(x)} \frac{\frac{1}{\tau_R^e} \left(\frac{1}{\tau_R^h} + \frac{1-f_M}{\tau_{MT}^e} + \frac{1-f_{F_n}(x_\varepsilon)}{\tau_{CBT}^e} \right) - \frac{1}{\tau_G^e} \left(\frac{1}{\tau_G^h} + \frac{f_M}{\tau_{MT}^e} + \frac{f_{F_n}(x_\varepsilon)}{\tau_{CBT}^e} \right)}{\frac{1}{\tau_R^e} + \frac{1}{\tau_G^e} + \frac{1}{\tau_G^h} + \frac{1}{\tau_R^h} + \frac{1}{\tau_{CBT}^e} + \frac{1}{\tau_{MT}^e}} D_t d\varepsilon, \quad (16)$$

$$U_{TAT}^{e(TUN)}(x) = \frac{d}{dx} \left[\int_{E_C(w)}^{E_C(x)} \int_{x_0}^{x_\varepsilon} \frac{\frac{f_{F_n}(x_\varepsilon)}{\tau_{CBT}^e} \left(\frac{1}{\tau_G^e} + \frac{1}{\tau_R^h} + \frac{1}{\tau_{MT}^e} \right) - \frac{1-f_{F_n}(x_\varepsilon)}{\tau_{CBT}^e} \left(\frac{1}{\tau_R^e} + \frac{1}{\tau_G^h} + \frac{f_M}{1-f_{F_n}(x_\varepsilon)} \frac{1}{\tau_{MT}^e} \right)}{\frac{1}{\tau_R^e} + \frac{1}{\tau_G^e} + \frac{1}{\tau_G^h} + \frac{1}{\tau_R^h} + \frac{1}{\tau_{CBT}^e} + \frac{1}{\tau_{MT}^e}} D_t dx \right] d\varepsilon. \quad (17)$$

and those for the tunneling escape times

$$(\tau_{CBT}^e(x, \varepsilon))^{-1} = (\tau_{TCB}^e(x, \varepsilon))^{-1} = \frac{m_R^e \sigma_t}{2\pi^2 \hbar^3} \int_{E_C(w)}^{\varepsilon} (\varepsilon - \varepsilon') \exp \left(-\frac{2}{\hbar} \int_x^{x_\varepsilon} \sqrt{2m_T^e (E_C(x) - \varepsilon')} dx \right) d\varepsilon' \quad (12)$$

$$(\tau_{MT}^e(x, \varepsilon))^{-1} = (\tau_{TMT}^e(x, \varepsilon))^{-1} = \frac{m_R^e \sigma_t}{2\pi^2 \hbar^3} \int_{E_V(x_0)}^{\varepsilon} (\varepsilon - \varepsilon') \exp \left(-\frac{2}{\hbar} \int_{x_0}^x \sqrt{2m_T^e (E_C(x) - \varepsilon')} dx \right) d\varepsilon' \quad (13)$$

where σ_t is the effective trap cross-section, m_R^e is the effective mass for calculating the Richardson constant in the semiconductor, m_T^e is the effective tunneling mass of electrons, $v_{th}^{e,h} = \sqrt{3kT/m_{e,h}^*}$ are thermal velocities of charge carriers, and w is the width of the space charge region. In terms of these escape times we derive the probability of occupation of the trap by electrons valid for the range of energies $\varepsilon \in (E_C(x_0), E_V(x_0))$:

$$f_t(x, \varepsilon) = \frac{\frac{1}{\tau_R^e} + \frac{1}{\tau_G^h} + \frac{f_{F_n}(x_\varepsilon)}{\tau_{CBT}^e} + \frac{f_M}{\tau_{MT}^e}}{\frac{1}{\tau_R^e} + \frac{1}{\tau_G^e} + \frac{1}{\tau_G^h} + \frac{1}{\tau_R^h} + \frac{1}{\tau_{CBT}^e} + \frac{1}{\tau_{MT}^e}} \quad (14)$$

Here, $x_{\varepsilon=E_C(x)}$ is the position of the intersection of energy level ε with $E_C(x)$, $f_{F_n}(x_{\varepsilon=E_C(x)})$ and f_M are the Fermi-Dirac distribution functions for electrons in the semiconductor and metal, respectively. By means of f_t one can express the two components of the electron recombination rates $U_{TAT}^{e(THER)}$ and $U_{TAT}^{e(TUN)}$, and U_{SRH} as integrals

$$U_{SRH}(x) = \int_{E_V(x)}^{E_C(x)} \frac{\frac{1}{\tau_R^e} \frac{1}{\tau_R^h} - \frac{1}{\tau_G^e} \frac{1}{\tau_G^h}}{\frac{1}{\tau_R^e} + \frac{1}{\tau_G^e} + \frac{1}{\tau_G^h} + \frac{1}{\tau_R^h} + \frac{1}{\tau_{CBT}^e} + \frac{1}{\tau_{MT}^e}} D_t d\varepsilon, \quad (15)$$

$$(16)$$

$$(17)$$

If we did not consider tunneling, it would mean that the tunneling escape times would be infinitely large and $1/\tau_{\text{CBT}}^e = 1/\tau_{\text{MT}}^e = 0$. Then the electron recombination rate $U_{\text{TAT}}^{e(\text{TUN})} = 0$, and $U_{\text{TAT}}^{e(\text{THER})}$ reduces to U_{SRH} . It should be also noted that if $\varepsilon < E_{\text{V}}(x_0)$, then in (14) to (17) the Fermi-Dirac distribution functions for electrons in the metal should be replaced by Fermi-Dirac distribution functions for holes in the semiconductor and the electron tunneling escape time τ_{MT}^e should be replaced by the hole tunneling escape time τ_{VBT}^h . This case is similar to a pn junction and the reader is referred to [7].

The electron recombination rate of direct tunneling is expressed as

$$U_{\text{DT}}^e(x) = \frac{dJ_{\text{DT}}^e(x)}{q dx} \quad (18)$$

where

$$J_{\text{DT}}^e(x) = \frac{qm_R^e}{2\pi^2\hbar^3} \int_{E_{\text{C}}(w)}^{E_{\text{C}}(x)} \exp\left(-\frac{2}{\hbar} \int_{x_0}^{x_g} \sqrt{2m_{\text{T}}^e(E_{\text{C}}(x) - \varepsilon)} dx\right) \times \left(\int_{\varepsilon/kT}^{\infty} (f_{\text{FM}}(\varepsilon', x_0) - f_{\text{Fn}}(\varepsilon', x_g)) d\varepsilon' \right) d\varepsilon \quad (19)$$

is the current of direct tunneling [8].

To solve the continuity equation it is required to define the boundary conditions. The Schottky boundary condition is associated with thermionic emission-diffusion transport theory (TED). The electron density at the maximum of the Schottky barrier at place x_0 , when the current is flowing, is

$$n(x_0) = \left[n_0 \left(v_{\text{TE}}^e + v_{\text{D}}^e \exp\left(\frac{qV_{\text{a}}}{kT}\right) \right) - v_{\text{D}}^e n_{\text{GR}} \right] / (v_{\text{TE}}^e + v_{\text{D}}^e) \quad (20)$$

$$\text{and } n_0 = N_{\text{C}} \exp(-\phi_{\text{b0}}/kT) \quad (21)$$

is the electron density at the maximum of the Schottky barrier in quasi-equilibrium, v_{TE}^e is the thermionic emission velocity given by $v_{\text{TE}}^e = (m_{\text{R}}^e k^2 T^2) / (2\pi^2 \hbar^3 N_{\text{C}})$, v_{D}^e is the effective diffusion velocity associated with the transport of electrons from the edge of the depletion layer at w to the potential energy maximum given by

$$\frac{1}{v_{\text{D}}^e} = \frac{q}{kT} \int_{x_0}^w \frac{1}{\mu^e(x)} \exp\left(\frac{\psi(x_0) - \psi(x)}{kT/q}\right) dx \quad (22)$$

$$\text{and } n_{\text{GR}} = \frac{q}{kT} \int_{x_0}^w \frac{\int_{x_0}^x U^e(x') dx'}{\mu^e(x)} \exp\left(\frac{\psi(x_0) - \psi(x)}{kT/q}\right) dx \quad (23)$$

is the effective recombination electron density associated with the generation-recombination process in the depletion layer. The hole density at the maximum of the Schottky barrier is

$$p(x_0) \cong p_0 = N_{\text{V}} \exp(-(E_{\text{g}} - \phi_{\text{b0}})/kT). \quad (24)$$

3. Simulation Results

The new TAT model was employed to simulate a Schottky diode prepared on a silicon doped GaN substrate with donor concentration $N_{\text{D}} = 2 \times 10^{18} \text{ cm}^{-3}$ and Schottky barrier height $\phi_{\text{b0}} = 1.2 \text{ eV}$. In GaN, the Huang-Rhys factor is $S = 6.5$ and the effective phonon energy $\hbar\omega_0 = 0.066 \text{ eV}$. The concentration of traps was assumed to be $N_{\text{t}} = 2 \times 10^{17} \text{ cm}^{-3}$. The distribution function D_{t} forms a band of traps at energy level $E_{\text{t}} = 0.7 \text{ eV}$ from the conduction band edge (see Fig. 2).

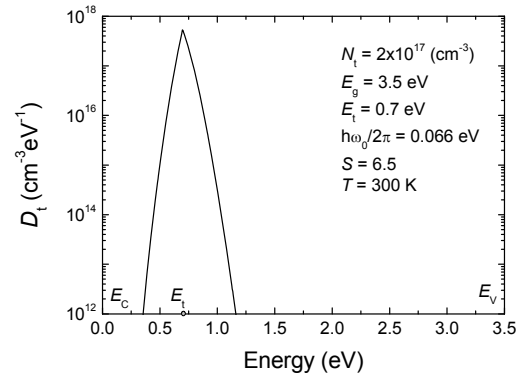


Fig. 2. The energy distribution function D_{t} of the traps in GaN. Huang-Rhys factor $S = 6.5$, effective phonon energy $\hbar\omega_0 = 0.066 \text{ eV}$, total trap concentration $N_{\text{t}} = 2 \times 10^{17} \text{ cm}^{-3}$, trap energy level $E_{\text{t}} = 0.7 \text{ eV}$ from the conduction band edge.

Effective masses $m_{\text{R}}^e = 0.2 m_0$ were used to evaluate the tunneling escape times τ_{CBT}^e and τ_{MT}^e . The tunneling probability was calculated using the WKB approximation and the effective masses were also set as $m_{\text{T}}^e = 0.2 m_0$. The ohmic contact at the back size of the structure was loaded by serial resistance $R_{\text{ohm}} = 5 \times 10^{-6} \Omega \text{ m}^{-2}$.

The I - V curves of such a Schottky structure were simulated at room temperature, $T = 300 \text{ K}$. The curves obtained for forward and reverse biased Schottky diodes are shown in Figs. 3 and 4, respectively. In the simulations we considered three various models of charge transport through the Schottky barrier:

- thermionic emission-diffusion model (TED),
- TED model along with direct tunneling (DT) between the metal and the conduction band of the semiconductor,
- TED model along with trap-assisted tunneling (TAT).

In addition, in all simulations we considered also Schottky barrier lowering caused by the image force. To demonstrate the influence of TAT upon the charge trans-

port we considered three different effective trap cross-sections, $\sigma_t = 10^{-20}$, 10^{-19} and 10^{-18} m^2 .

The simulated I - V curves prove that the TAT mechanism of charge transport dominates in a reverse biased Schottky structure, whereas in a forward biased structure the dominant mechanism of charge transport is direct tunneling, DT. Naturally, an increased effective trap cross-section σ_t and density of traps N_t lead to a higher contribution of trap-assisted tunneling, while direct tunneling remains intact. Simulations of I - V curves of real Schottky diodes require simultaneous consideration of the three mechanisms of charge transport, thus TED + DT + TAT.

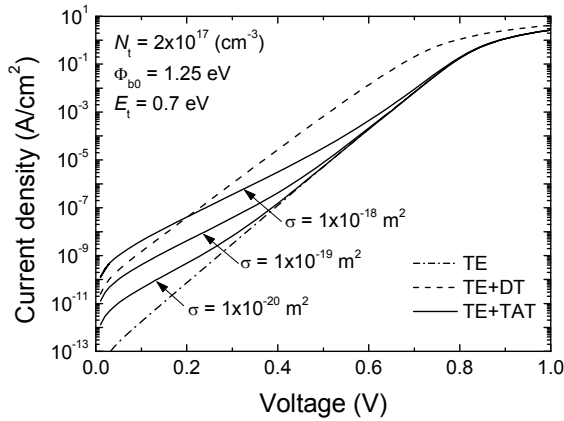


Fig. 3. Forward I - V curves of Schottky diodes on GaN with different models of charge transport through the Schottky barrier.

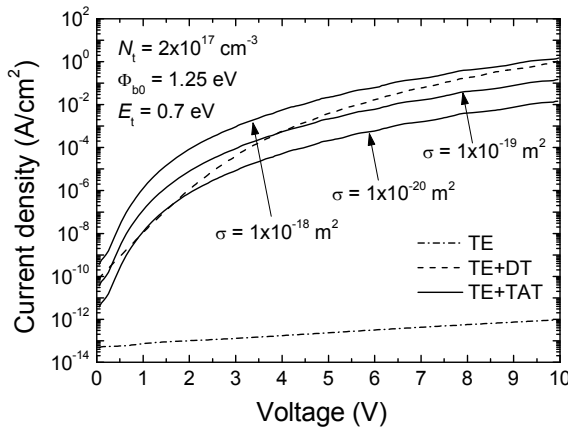


Fig. 4. Reverse I - V curves of Schottky diodes on GaN with different models of charge transport through the Schottky barrier.

4. Conclusions

The presented TAT model of charge transport aims at explaining the origin of large leakage currents in reverse biased Schottky diodes shutting the 2D channel in high electron mobility transistors (HEMTs). It is obvious that multiphonon broadening of the band of traps together with trap-assisted tunneling markedly affect the I - V curves of

the diodes. The new TAT model has the ability to describe the generation and recombination as well as the tunneling processes in Schottky junctions.

List of Symbols

D_t	distribution of traps
$E_{C,V}$	bottom of the conduction band or top of the valence band
E_F	Fermi level in the metal
E_g	energy bandgap
E_t	energy level of the trap
f_B	Bose distribution function
f_{Fn}	Fermi-Dirac distribution function for electrons in the semiconductor
f_{Fm}	Fermi-Dirac distribution function for electrons in the metal
f_t	occupation probability of trapping centers at energy ε
J_D^e	electron drift-diffusion current density
J_D^h	hole drift-diffusion current density
k	Boltzmann constant
$m_{e,h}^*$	effective masses of electrons and holes
m_R^e	electron mass for calculating the Richardson constant
m_T^e	effective tunneling mass of electrons
m_0	electron mass
n	concentration of free electrons
n_0	electron density at the maximum of the Schottky barrier
n_{GR}	effective recombination electron density
$N_{C,V}$	effective density of states in the conduction or valence band
$N_{A,D}$	donor and acceptor dopant density
N_D^+	concentration of shallow ionized donors
N_t	density of traps
N_t^+	concentration of deep ionized traps
p	concentration of free holes
p_0	concentration of holes at the maximum of the Schottky barrier
q	elementary charge
S	Huang-Rhys factor
T	absolute temperature
U^e	overall generation-recombination rate
U_{DT}^e	rate of direct tunneling
U_{SRH}	Shockley-Read-Hall generation-recombination rate
$U_{TAT}^{e(THER)}, U_{TAT}^{e(TUN)}$	two components of trap-assisted generation-recombination rates
V_a	applied voltage
w	width of the space charge region
x	coordinate perpendicular to the interface
x_e	position of intersection of energy level ε with $E_C(x)$
x_0	position of the metal-insulator interface
\hbar	reduced Planck constant, $\hbar/2\pi$

ε	electron energy
ε'	electron energy in the direction of tunneling
ε_r	lattice relaxation energy
κ	semiconductor permittivity
ϕ_{b0}	Schottky barrier height
$\mu^{e,h}$	electron or hole mobility
$v_{th}^{e,h}$	thermal velocity of electrons or holes
v_{TE}^e	thermionic emission velocity
v_D^e	effective diffusion velocity of electrons
σ_t	effective trap cross-section
τ_R^e	escape time characterizing the recombination of free electrons, thus capturing of electrons by the trapping center
τ_R^h	time of recombination of holes
τ_G^e	time of generation of free electrons, thus emission of electrons from the trapping center to the conduction band
τ_G^h	time of generation of holes
$\tau_{CBT}^e, \tau_{TCB}^e$	time of tunneling of electrons from the conduction band to the trap and vice versa
τ_{MT}^e, τ_{TM}^e	time of tunneling of electrons from the metal to the trap and vice versa
τ_{VBT}^h	time of tunneling of holes from the valence band to the trap
ψ	electrostatic potential
$\hbar\omega_0$	effective phonon energy

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References

- [1] MIMOUNI, A., FERNÁNDEZ, T., RODRIGUEZ-TELLEZ, J., TAZON, A., BAUDRAND, H., BOUSSUIS, M. Gate leakage current in GaN HEMT's: A degradation modeling approach. *Electrical and Electronic Engineering*, 2012, vol. 2, no. 6, p. 397 - 402.
- [2] YAMADA, T., TSUCHIYA, T., IMADA, K., IWAMI, M., KIKAWA, J., ARAKI, T., SUZUKI, A., NANISHI, Y. Gate leakage currents of AlGaIn/GaN HEMT structures grown by metalorganic vapour phase epitaxy. *Physica Status Solidi (c)*, 2007, vol. 4, no. 7, p. 2690 - 2694.
- [3] HOUSSA, M., TUOMINEN, M., NAILI, M., AFANAS'EV, V., STESMANS, A., HAUKKA, S., HEYNS, M. M. Trap-assisted tunneling in high permittivity gate dielectric stacks. *Journal of Applied Physics*, 2000, vol. 87, no. 12, p. 8615 - 8620.
- [4] RACKO, J., MIKOLÁŠEK, M., GRANZNER, R., BREZA, J., DONOVAL, D., GRMANOVÁ, A., HARMATHA, L., SCHWIERZ, F., FRÖHLICH, K. Trap-assisted tunneling current in MIM structures. *Central European Journal of Physics*, 2011, vol. 9, no. 1, p. 230 - 241.
- [5] RACKO, J., MIKOLÁŠEK, M., HARMATHA, L., BREZA, J., HUDEC, B., FRÖHLICH, K., AARIK, J., TARRE, A., GRANZNER, R., SCHWIERZ, F. Analysis of leakage current mechanisms in RuO₂-TiO₂-RuO₂ MIM structures. *Journal of Vacuum Science and Technology B*, 2011, vol. 29, no. 1, p. 01AC08-1 - 01AC08-8.
- [6] SCHENK, A. A model for the field and temperature dependence of Shockley-Read-Hall lifetimes in silicon. *Solid-State Electronics*, 1992, vol. 35, no. 11, p. 1585 - 1596.
- [7] RACKO, J., MIKOLÁŠEK, M., GRMANOVÁ, A., BREZA, J., BENKO, P., GALLO, O., HARMATHA, L. A new model of multiphonon excitation trap-assisted band-to-band tunneling. *Radioengineering*, 2012, vol. 21, no. 1, p. 213 - 218.
- [8] RACKO, J., MIKOLÁŠEK, M., GRANZNER, R., AL MUSTAFA, N., SCHWIERZ, F., BREZA, J. The impact of changed barrier layer parameters upon tunnelling in GaN/AlGaIn/GaN Schottky structures. In *Proceedings of the 9th International Conference on Advanced Electron Devices and Microsystems ASDAM 2012*. Smolenice (Slovakia), 2012, p. 207 - 210.

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